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LCA OF CHEMICALS

REACH and LCA—methodological approaches and challenges

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Abstract
Purpose This paper discusses issues associated with the research question: What are the similarities and differences between the REACH and life cycle assessment (LCA) approaches, and how can synergies between these two approaches be exploited to achieve environmental improvements in a holistic perspective?
Methods The Innochem project (Hanssen 2010) has been the vehicle for examining two different approaches for product improvement: REACH and LCA. Product LCAs and REACH assessments were performed on several products from each of the two main company participants, i.e. Jotun and HÅG. These companies are downstream users, according to the REACH definition: Jotun producing mixtures and HÅG manufacturing articles. Knowledge of the REACH and LCA aspects associated with these two types of products existed in the project team and was used in the project period (2006–2011) to compare the two approaches.
Results This paper presents similarities and differences between REACH and LCA approaches as related to reducing impacts on the environment. As an illustrative example, the REACH registration dossier is compared to USEtox data for benzene.
Conclusions Combining aspects of LCA with REACH can give companies a competitive edge and benefit society. The greater availability of toxicity data that will result from REACH can strenghten LCA toxicity assessments and methods. The functional life cycle approach and potential synergies from LCA are important when implementing REACH in companies in order to avoid suboptimal solutions and exploit the potential for achieving innovative improvements. Many companies will use both approaches, which may lead to results pointing in the same direction, or contradictory results. Using both approaches and exploiting concurrence and synergies between them will ensure that decision makers are aware of potential conflicts during the product development process and can thus be able to seek solutions that will avoid these conflicts of interest.

Keywords Chemicals · Environmental improvements · LCA · Products · REACH

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1 Introduction

Companies developing existing and new products in Europe today need to consider both regulatory requirements and environmental performance during their product development processes. In this paper the author will look more closely at life cycle assessment (LCA) and the REACH directive, which are two different approaches aiming at improving the environmental performance of products.

ISO 14044 describes LCA as a technique for better understanding and addressing the environmental impacts associated with products and services. LCA is a standardised method that has a clear focus on the function for the user of the product or service, with the intention of minimising total impacts on the environment occurring as a result of fulfilling this function. Results from LCA studies used for product or system improvements have shown that it is not always the case that all impacts can be reduced by a given improvement option (Modahl et al. 2008, 2009;

WRAP 2006; Hertwich et al. 2008). There can be trade-offs between environmental impacts, e.g. reducing global warming potential, but increasing other environmental impacts like acidification or toxic impacts or vice versa (Wenzel et al. 2008; Høibye et al. 2008). These potential trade-offs highlight the need to consider product and product system changes in a holistic and functional perspective; if this need is ignored, then supposed improvements may have unintended and even counterproductive consequences.

REACH stands for Registration, Evaluation, Authorisation and Restriction of Chemicals. The REACH directive was adopted by the European Union (EU) in December 2006 and requires companies importing or producing chemicals (>1 t/year) in the EU and EEA[1] regions to register these chemicals with the EU's Chemicals Agency (ECHA). The requirements of REACH are relevant for both individual substances and substances in mixtures (e.g. paint), although the registration demand is for substances only. REACH requires companies to register the substance's identity, classification and labelling, test results and proposed further tests for the substance, exposure potential to humans and different environmental compartments, and recommendations for safe use. The requirements for REACH increase with increased quantities of chemicals imported or produced. If a company operates with quantities greater than 10 t/year/producer or importer, a risk assessment ("chemical safety report", CSR) is required for the substance. If a chemicals company does not comply with REACH, it cannot sell the particular products on the European market.

The requirements of REACH impose a large burden of documentation on industry, and the Innochem project is part of the Norwegian work towards assisting companies in approaching the new REACH requirements and dealing with these in the most efficient manner possible. The Innochem project (Hanssen 2010) aims at turning new regulations for chemicals into a promoter of innovation instead of being a threat to research and development, innovation and production of chemicals in Norway and Europe. Innochem is a collaborative project involving companies (Jotun A/S and HÅG as) and research institutions (Ostfold Research, NIVA, UiO, NTNU and Aalborg University) financed by the Norwegian Research Council (BIA programme, Brenna 2010) and participating companies. As part of the Innochem work, it is important to establish the similarities and differences in the methodological approaches used in REACH and LCA. This paper will endeavour to shed light on these issues.

[1] European Economic Area

2 The REACH regulation

Historical developments in legislation and international cooperation leading up to the REACH regulation are well described in Løkke (2004). The Organisation for Economic Co-operation and Development took a leading role in developing international consensus on good laboratory practice (GLP) and testing procedures. This work from the 1980s has also been an important basis for the division of labour and schedules of tests that is reflected in the REACH regulation today. Growing concern about the long-term effects of chemicals meant that the desire for early warning and prevention of these unforeseen effects and the use of the precautionary principle as the basis for chemicals regulation arose (Løkke 2004). Developments in occupational health regulations internationally were also important for the development of REACH, in order to minimise the adverse effects on the health of workers producing and using chemicals.

REACH entered into force on 1 June 2007 to streamline and improve the EU's former legislative framework on chemicals. REACH places the responsibility on industry to carry out chemical safety assessments (CSA) and manage the risks that chemicals may pose to human health and the environment. The aims of REACH are (ECHA 2010a; Van Leeuwen and Vermeire 2007): to improve the protection of human health and the environment from the risks that can be posed by chemicals; to enhance the competitiveness of the EU chemicals industry, a key sector for the economy of the EU; to promote alternative methods for the assessment of hazards of substances and to ensure the free circulation of substances on the internal market of the EU.

3 Background on LCIA methods

Life cycle assessment is carried out in phases (ISO 14044 2006; European Commission 2010a, b; Baumann and Tillman 2004): goal and scope definition, inventory analysis, impact assessment and interpretation. Section 4 of this paper will refer to different life cycle impact assessment (LCIA) methods that include toxic impacts, specifically USEtox™ and ReCiPe. This section of the paper will therefore give a brief introduction to these methods and relevant references.

USEtox™ is described as a consensus model for chemical impact characterisation related to human toxicity and freshwater ecotoxicity (Rosenbaum et al. 2008) and is a result of the United Nations Environment Programme (UNEP)-Society for Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative. Pizzol et al. (2010) provides an overview figure of different existing LCIA methodologies. This overview shows that USEtox™

builds upon EcoIndicator 1999 (Goedkoop and Spriensma 2000), Impact 2002+ (Jolliet et al. 2003), Environmental Design of Industrial Products (EDIP) 97 (Wenzel et al. 1997; Hauschild and Wenzel 1998) and TRACI (Bare et al. 2003). As described in Pizzol et al. (2010), USEtox™ is not a complete, stand-alone, LCIA method, as it includes only human and ecotoxicity, but it is a multimedia model that can assess both fate and exposure for a number of chemical emissions.

ReCiPe is a method that, like EcoIndicator 99, offers end-point results for a set of environmental damages and weights results based on the decisions of a panel of experts (Wernet et al. 2010). The acronym ReCiPe is appropriate because the method provides a recipe to calculate life cycle impact category indicators; it also represents the initials of the institutes that were the main contributors: RIVM and Radboud University, CML and PRé (Goedkoop et al. 2009). Pizzol et al. (2010) describes ReCiPe as harmonizing the two Dutch models CML2001 and EcoIndicator 99, linking the midpoint approach in CML 2001 with the end-point approach in EcoIndicator 99 in a consistent way. ReCiPe does this in two steps, so that the user can choose where to end their analysis [midpoint, e.g. for human toxicity kilograms 1,4-dichlorobenzene equivalents, or end-point level, e.g. disability-adjusted life years (DALY)].

The Uniform System for the Evaluation of Substances (USES)-LCA is a nested multimedia model for fate, exposure and effects (Huijbregts et al. 2000). The CML 2001 method was based on this model. USES-LCA was developed by adapting USES 2.0 to meet LCA-specific demands, which are described in Huijbregts et al. (2000). As described in Van Beelen (2000), USES was developed by the National Institute of Public Health and the Environment (RIVM) in the Netherlands to evaluate the potential hazards and risks of notified substances on the basis of a specified dataset. The European Union System for the Evaluation of Substances (EUSES) was developed based on USES 1.0 and the European Union Technical Guidance Document (EC 1996). Both USES and EUSES risk assessment systems are available in computerised form, where the user enters chemical properties and assumptions about the use of the chemical in order to obtain risk assessment data for the chemical for both man and the environment (Van Beelen 2000).

4 Similarities and differences between REACH and LCA

This section of the paper compares the similarities and differences between REACH and LCA approaches and also includes discussion of these, as a basis for the conclusions in the final part of the paper. For this comparison and discussion, the paper focuses on the following topics:

- Goal and scope
- Function and functional unit
- System boundaries
- Data collection (inventory)
- Impact assessment
- Interpretation and application

These topics were chosen because they highlight the differences between the two approaches as well as the areas where the author sees the potential for synergies that could contribute to minimisation of adverse impacts from products and services. The areas focussed upon here will be an important basis for further work towards developing tools that can be efficiently exploited by companies wishing to be proactive with their product develpment work. LCA practitioners will also be familiar with the terminology used to structure this chapter, as this reflects terminology used in LCA methodology and standards.

Benzene has been used as an example to illustrate the similarities and differences described in this chapter. Each subsection contains information about how the relevant aspects are approached using an LCA or a REACH approach. Benzene has been chosen as it has a REACH registration dossier (ECHA 2011a) and is incorporated into USEtox. The USEtox characterisation factors for benzene are described as “recommended” and not interim (USEtox™ 2010a). Benzene is an example (with readily available data and references) that is generally applicable, as the data sources are those that should be available (via ECHA) for all REACH registered substances after the registration deadlines.

4.1 Goal and scope

REACH is an EU regulation based on risk assessment. Risk assessment involves gathering and evaluating data on health and or environmental effects and disease which can be caused by a chemical under specific exposure conditions. These data are based on experimental evidence of damage, injury or disease, which is either directly applicable to the species and relevant exposure conditions or extrapolated from relevant studies on other species and/or exposure conditions (Van Leeuwen and Vermeire 2007). Whereas LCA is a standardised method for documenting the *potential* environmental impacts associated with products and services, which is used as a decision support tool. Adherence to REACH is compulsory for companies producing or importing chemicals in the EU (“No data, no market”, Article 5, Commission of the European Communities 2007). LCA is however not mandatory but is an internationally standardised methodology which, as well as being important in its own right, is also used as a basis for Environmental

Product Declarations (EPDs), ecolabels, carbon footprint, etc. Thus it does not seem obvious that these two approaches have many similarities at all. However, both approaches intend to minimise impacts on the environment. LCA has focus on products and services and includes evaluation of the potential environmental impacts associated with these (ISO 14044 2006). Many companies will attempt to use both approaches as part of environmental analysis and might find that the conclusions from the two approaches are sometimes contradictory.

LCA methodology is also often used by companies in order to focus on improvements for product systems (Baumann and Tillman 2004). This is an aspect of LCA methodology that could provide positive influence on REACH implementation by contributing to an innovative improvement perspective.

The following describes the comparison of goal and scope aspects for the benzene example. The example is for a company that requires the LCA as the basis of an EPD for benzene (falling under the PCR for basic organic chemicals, EPD 2011) to document the environmental profile of benzene for sale in the European market. Currently EPDs do not include toxic effect indicators (Abrahamsen et al. 2008), but the company commissioning the study also wishes to include toxic effects in the LCA study. The LCA is a cradle-to-gate study, including extraction of raw materials (crude oil), processing, production and on-site storage of benzene, prior to transport to the customer. The study is also to be used for the company's internal learning purposes, identifying the largest environmental impacts and future improvement options. In this case, the specific producer, manufacturing site and composition of the product (i.e. if not 100% pure benzene) would be declared and included in the goal and scope. In order to compare this to the REACH approach, the registration dossier for benzene has been consulted (ECHA 2011a). Figure 1 shows a screenshot of the menu for the registration dossier. This menu includes "Manufacture, Use and Exposure", but this section contains "Identified uses", information on uses ("by workers in industrial settings") and the process category, and sector in which it is used. The older International Uniform Chemical Information Database for benzene (European Commission 2010a) listed all the producers and importers of benzene in Europe, including their addresses and telephone numbers. This information is not present in the registration dossier, but information about producers of given chemicals is publicly available from other sources. The European Pollutant Release and Transfer Register can be consulted if contact information is wanted for emitters of benzene in Europe (EEA 2011a) or different types of industrial activity (i.e. the location of industrial scale production of basic chemicals that produce simple cyclic hydrocarbons, EEA 2011b).

4.2 Function and functional unit

The REACH regulation applies to chemicals on a tonnage basis, whereas LCA has a functional and life cycle focus. In REACH, the "function" of a chemical is interpreted as a description of its use. By contrast, the "function" in LCA is the purpose that the product is designed to fulfil; it is then possible to calculate the amounts of materials and chemicals required (reference flows in LCA terminology). The potential hazards associated with chemicals and the amounts produced, or imported, determine the level of documentation and testing required for the REACH approval of their use by ECHA.

In LCA, the functional unit is defined as the "quantified performance of a product system for use as a reference unit" (ISO 14044 2006). The functional unit is part of the scope of the study and provides a reference to which the input and output data are normalised. LCA approaches the environmental impacts of products and services with a clear focus on the function for the user (ISO 14044 2006; Baumann and Tillman 2004). REACH is concerned with quantities of chemicals and their properties, independent of the amount needed to fulfil a function over a period of time. The functional approach is essential when considering substitution of a given chemical, or substance. It is possible that a substitute chemical has lower toxic impacts per kilogram, but more of it is required in order to fulfil the same function. In such cases, substituting one substance with another that seems to be less hazardous can lead to a total increase in environmental impacts throughout the life cycle, when the functional perspective is included. As long as the substitute substance is already approved for the particular use, the demand for exposure scenarios in order to fulfil REACH requirements would not be affected. If the chemical is significantly less hazardous, the demand for exposure scenarios could in fact be reduced. It is therefore vital that the life cycle approach is considered together with the implications of REACH in order to ensure real improvements in the functional and holistic environmental profiles of products used in society. Without this approach, supposed improvements may be suboptimal or even counterproductive.

The benzene example was used to consider the functional unit aspect in the REACH approach compared to the LCA approach. The registration dossier for benzene does not specify the volume (ECHA 2011a) but implies production or importation to the EU in a quantity sufficient to require such a dossier. The description of uses (REACH function) of benzene included in the dossier is described in Section 4.1. For an LCA of the basic chemical benzene, the funtional unit is 1,000 kg of packaged product ready for delivery (EPD 2011).

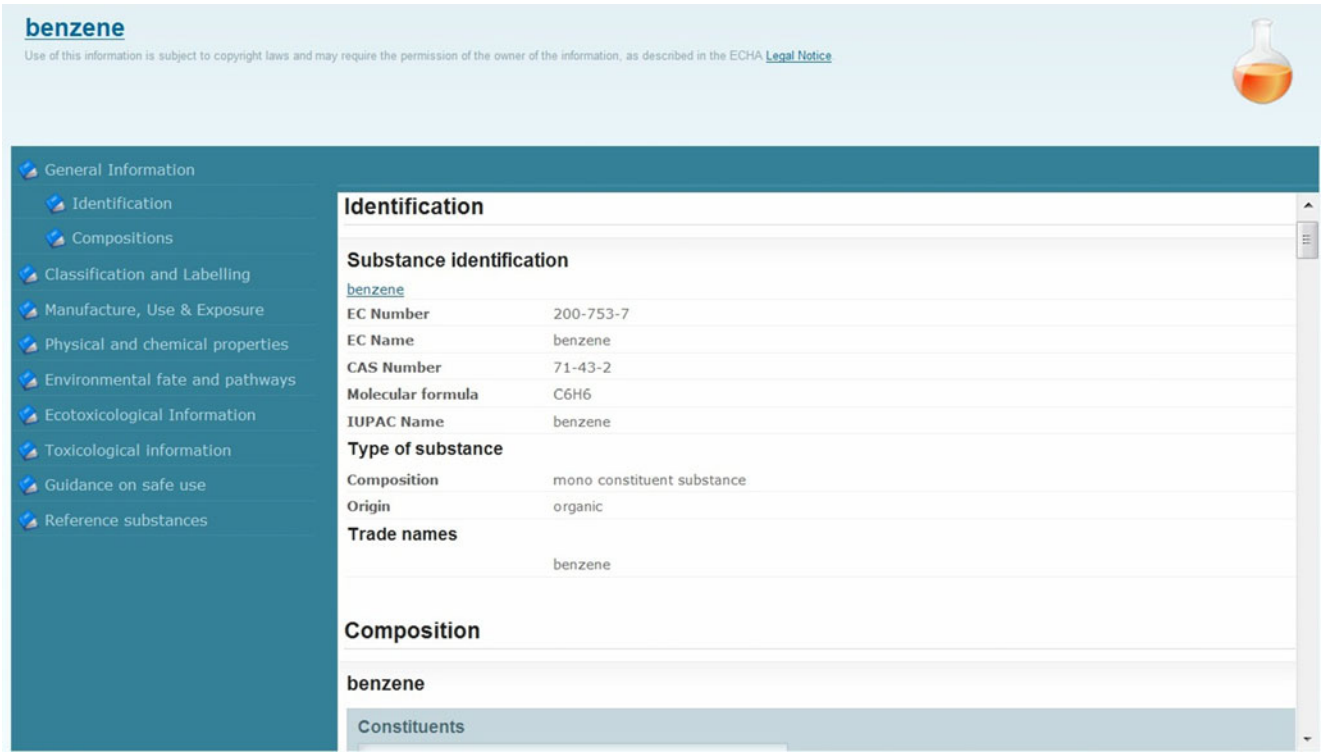

Fig. 1 Benzene registration dossier screen picture. Source: European Chemicals Agency (http://echa.europa.eu/)

4.3 System boundaries

The goal and scope of the study in LCA affect the system boundaries. In LCA, system boundaries include which unit processes should be included in the study and the level of detail to which they are to be studied. This description often includes a flow diagram of the product life cycle, clearly showing which life cycle stages are included in the study (ISO 14044 2006). The REACH regulation includes the term "life cycle" in a different context: there, it refers to the life cycle of the chemical substance from manufacture and use, followed by release into the environment and its progress through the ecosystem. In the toxicological information required for REACH chemical safety assessments, the term life cycle is relevant in terms of the life cycle of the organisms affected by the chemical in question (e.g. developmental toxicity). In LCA, the life cycle of the product concerns the value chain of processes and logistical interactions that are needed in order to produce and use the product during its lifetime. For example, this could include extraction of raw materials and resources needed to produce the product, production of intermediates, production and use of the product itself (including maintenance) and its final disposal, or recycling. Ideally, LCA studies include all the relevant inputs and outputs from this value chain (e.g. electricity consumption and direct emissions) as well as the indirect resource consumption and indirect emissions associated with these inputs and outputs (e.g. emissions to air from coal power, where electricity from coal is an input to a given process in the relevant value chain). REACH does not encompass resource consumption and emissions arising from the production of chemicals. Intermediate products are only considered if they are on-site isolated intermediates or if they are transported in quantities over 1 t or more per year (Commission of the European Communities 2007).

System boundaries in LCA also include the selection of impact categories, category indicators and characterisation models. These categories can include many different environmental impacts, such as global warming potential, ozone depletion potential and acidification potential, as well as potential toxic effects on humans and the environment. REACH is concerned with toxic impacts on humans and the environment and does not directly include other environmental effects. However, it is interesting to note that in ECHA (2008), LCIA is given as useful in order to get an idea of likely resulting impacts "in the case several emissions not related to (eco)toxicity have been identified".

The following compares system boundary aspects for the two approaches. The benzene example system boundaries for the LCA study would be based on an attributional approach (as appropriate for an EPD, Baumann and Tillman 2004, European Comission 2010a, b). The product system to be studied would be cradle to gate; the PCR for chemical

products would be followed. Downstream processes (use and disposal) would not be qualitatively included in the EPD (2011). The data for core modules would be representative for the actual processes on the given production site, within the time frame for which the EPD is valid (maximum 3 years). In practise, this often means the last calendar year for which production data are available. Boundaries to nature are defined as material and energy resource flows from nature into the system. The life cycle inventory cut-off rules are specified in the PCR as "a minimum of 99% of total inflows regarding energy, mass, and environmental relevance, to the core module shall apply." It is not mandatory to declare any quantative information about use and end-of-life phases, but a short description of the main applications and associated disposal scenarios should be declared. This should include a qualitative description of "key environmental aspects associated with the use and end-of-life fate" of the product.

The registration dossier for benzene does not describe the chemical life cycle or the way it affects the life cycle of test organisms in detail. It does, however, provide the results of available test data for benzene. The available data include reproductive toxicity, environmental toxicity, many other types of test as well as the physico-chemical properties of benzene. Examples of some of the data given in the registration dossier are included in Table 1.

4.4 Data collection (inventory)

In order to perform the assessments required, experts have to quantify emissions to the environment and potential impacts on the environment and human health associated with these. Both approaches also require considerable amounts of data collection and management. If a produced product falls under REACH, the information required for general registration is detailed in annex VI of the regulation (Commission of the European Communities 2007). This includes the following: general registrant information, identification of the substance (including physical and chemical properties), information on its manufacture and use, classification and labelling (e.g. hazard classification), guidance on safe use [including first-aid and risk management measures (RMM)] and information on exposure. If a substance is manufactured or imported in quantities of 10 t or more, detailed information is required, specifically toxicological information (described in annex VIII of the regulation, e.g. skin irritation, eye irritation and mutagenicity). The level of toxicological information and the type of data required increases for chemicals produced in quantities over 100 t per year (e.g. repeated dose toxicity, reproductive toxicity and ecotoxicological information, annex IX) and also for those produced over 1,000 t per year (e.g. carcinogenicity, annex X).

Release estimation for REACH environmental exposure estimation is not based on the physico-chemical properties of the substance, but the substance properties are used as an important part of the environmental exposure estimation. This is fully in line with the LCIA approach [e.g. USEtox™ (Rosenbaum et al. 2008; Hauschild et al. 2008) and USES-LCA (Van Zelm et al. 2009b)].

There is an equivalent process in LCIA to the process in REACH of estimating releases: this is the life cycle inventory phase, which maps the emissions released into the environment. This information is often obtained from companies and/or databases. If unknown, the REACH guidance (in its current form) recommends default parameters for derivation of the environmental release rate. A table of default values is given in regulations (Table R.16-23, ECHA 2010b), where values are given for default worst case release factors, e.g. manufacture of chemicals: 5% to air, 6% to water (before sewage treatment plant) and 0.01% to soil. The values shown in this table have been selected from general release information from EC (2003) for representative cases but assuming there are no risk management measures in place. The distribution of the chemicals in question is not based on physico-chemical properties of a substance. The guidance describes these values as conservative.

Exposure scenarios for workers required under REACH will include intake fraction estimates. Exactly the same estimates can have direct application in LCIA human toxicity work, e.g. in the USEtox methodology CF=iF× EF, where CF (cases/kilogram$_{emitted}$) is the characterisation factor, iF is the intake fraction (kilogram$_{intake}$/kilogram$_{emitted}$) and EF is the effect factor (cases/kilogram$_{intake}$, Hauschild et al. 2008; Rosenbaum et al. 2008; Hellweg et al. 2009).

Implementation of REACH will lead to greater availability of toxicity data for chemicals and substances in use in Europe. This can strengthen LCA results and methodology by providing useful data for evaluation of toxic effects in a life cycle perspective. A major problem with using existing methods for toxic effects (both for humans and ecosystems) in LCA has been data availability and data quality. This is both in terms of inventory data and chemical fate and effect data regarding assessment models. An illustration of this is that SimaPro 7.3.0 (PRé Consultants 2011), a well-known LCA tool, including several LCA databases, that includes less than 4,000 different substances that can be emitted to air and less than 3,500 that can be emitted to water. The USEtox database (USEtox™ 2010a, b) includes CFs for 3,073 organic and 21 inorganic substances. Uncertainties associated with models used for the evaluation of the potential human health and ecotoxicity impacts used in LCA have been discussed by many authors, some examples being Reap et al. (2008), Larsen and Hauschild (2007), Huijbregts et al. (2003) and Van Zelm et al. (2006, 2009a).

Table 1 Data for benzene in the USEtox model compared with the REACH Registration Dossier

Data	USEtox	REACH registration dossier
Identification number	CAS number: 71-43-2	EC number: 200-753-7 CAS number: 71-43-2
Name	Benzene	Benzene
Molecular weight (g mol^{-1})	78.1	78.1118
Octanol/water partition coefficient (K_{ow})	135	log K_{ow} 2.13 (K_{ow}=135)
Organic carbon normalised solids–water partition coefficient (K_{oc})	56.2 l/kg	100–900 l/kg
Henry coefficient (K_H25C)	561 Pa m^3/mol	
Vapour pressure	12,600 Pa (25°C)	10 kPa at 20°C and 100 kPa at 79.7°C
Solubility	1,790 mg/l (25°C)	circa 1.88 g/l at 23.5°C
Degradation in air (k_{degA})	9.23 E-07 s^{-1}	
Degradation in water (k_{degW})	2.14 E-07 s^{-1}	
Degradation in soil (k_{degSd})	2.38 E-08 s^{-1}	
Degradation in sediment (k_{degSl})	1.07 E-07 s^{-1}	
Distribution modelling		Air / Water (fresh) / Soil / Sediment Concentration: 2.1 μg/m^3 / 58 ng/l / 12 ng/kg / 130 ng/kg Distribution (%): 99.0 / 0.9 / 0.1 / 0.1 Removal by reaction (%): 4.6 / 0.2 / n.c. / n.c. Removal by advection (%): 95.2 / 0.1 / n.c. / n.c. *n.c.* not calculated "Transportation through the air seemed to be the most important removal mechanism."
Average log EC50	1.51 mg/l	
Toxicity, inhalation	ED50 inhalation, non-cancer 135 kg $lifetime^{-1}$ (ED50=the chronic dose of a substance with mode of action affecting 50% of the human population)	Repeated dose toxicity, inhalation: "Repeated inhalation exposure to benzene at 6 h/day, 5 days/week produces haematotoxicity in mice. The NOAEC [no observed adverse effect concentration] was 10 ppm (32 mg/m^3)." Toxicity to reproduction: "Exposure of adult female Sprague–Dawley rats to benzene via inhalation at concentrations up to 300 ppm (960 mg/m^3) in a one-generation reproduction study produced no evidence of toxicity, body weight, and/or altered reproductive performance. There were no treatment-related effects on pup survival, or gross pathology and no significant adverse effects on body weights or organ weights. An exposure concentration of 300 ppm (960 mg/m^3) is a NOAEC for both adult and offspring toxicity and female fertility."
Toxicity, oral	ED50 ingestion, non-cancer 135 kg $lifetime^{-1}$	Repeated dose toxicity, oral: "Repeat oral administration of benzene to rats is associated with adverse effects in the haematopoietic system. NOAEL [no observed adverse effect level] for males was 200 mg/kg. No NOAEL was established for females. LOAEL for females was 25 mg/kg/day (lowest dose tested)."
Carcinogenic effects, inhalation	ED50 inhalation, cancer 34.1 kg $lifetime^{-1}$	Reproductive toxicity: "Exposure of adult female Sprague–Dawley rats to benzene via inhalation at concentrations up to 300 ppm (960 mg/m^3) in a one-generation reproduction study produced no evidence of toxicity, body weight, and/or altered reproductive performance. There were no treatment-related effects on pup survival, or gross pathology and no significant adverse effects on body weights or organ weights. An exposure concentration of 300 ppm (960 mg/m^3) is a NOAEC for both adult and offspring toxicity and female fertility." Genetic toxicity in vivo: "Benzene produced an increased frequency of micronuclei following inhalation exposure in mice and is considered to be an in vivo clastogen."

Table 1 (continued)

Data	USEtox	REACH registration dossier
Carcinogenic effects, ingestion	ED50 ingestion, cancer 34.1 kg lifetime^{-1}	Three sets of key data are given (including doses and results). The conclusions are: "Benzene is carcinogenic in mice following oral exposure at=25 mg/kg for 2 years. Increased tumour incidences were seen in multiple tissues. A NOAEL was not determined." "Benzene is carcinogenic in rats following oral exposure. Increased tumour incidences were seen in the Zymbal gland, oral cavity and skin." "Benzene inhalation at 300 ppm (960 mg/m^3) for 6 h/d, 5 d/week for 16 weeks was carcinogenic in C57Bl/6 female mice. There was an increased incidence of lymphoma/ leukaemia and Zymbal gland and ovarian tumours."
BAF fish	4.27 lkg^{-1} fish	
PNEC aqua (freshwater)		1.9 mg/l
PNEC aqua (marine)		1.9 mg/l
PNEC sediment (freshwater)		33 mg/kg sediment dw
PNEC soil		4.8 mg/kg soil dw
Acute toxicity: oral		"Acute oral toxicity was determined in groups of at least 6 rats per age and dose level. Benzene was demonstrated to be of low acute oral toxicity (LD50 [dose of a toxicant lethal to 50% of the test population] >2,000 mg/kg) and does not warrant classification under Dir 67/548/EEC or GHS"
Acute toxicity: inhalation		"The acute inhalation LC50 of benzene was determined in groups of 10 or 12 female rats to be 13,700 ppm (43,767 mg/m^3; 43.7 mg/l) with a range of 13,050–14,380 ppm (41,690–45,939 mg/m^3). Death appeared to be caused by a depression of the CNS. These animals had increased lung and liver weights, lung and liver congestion and an increased number of vacuolated hepatocytes in the liver." "Benzene is of low acute inhalation toxicity and does not warrant classification under Dir 67/548/EEC."
Acute toxicity: dermal		"The acute dermal LD50 for benzene was determined in groups of 4 rabbits (abraded skin) or guinea pigs (abraded back skin or non-abraded abdominal skin) using occlusive dressings." "The acute dermal LD50 was >9.4 ml/kg (8,260 mg/kg) in each case." "In conclusion, benzene is of low acute dermal toxicity and does not warrant classification under Dir 67/548/EEC or GHS."

BAF bioaccumulation factor, *dw* dry weight, *PNEC* predicted no effect concentration

This issue is also addressed in the literature about the UNEP-SETAC Life Cycle Initiative consensus work (e.g. Rosenbaum et al. 2008; Hauschild et al. 2008). The increased focus on toxic effects and amounts of chemicals and substances in society should make it easier to obtain these data. In this way data arising from REACH may help to fill the gaps for chemicals and substances that do not have characterisation factors in current toxic effect models. Thus, both REACH and LCA may benefit by exploiting information and data from each other's guidance documents and databases. One example of this is in ECHA (2008, p. 75), where it is written that "LCA databases may provide average emission data related to the impacts of various materials and processes" (required for social economic analysis).

Models developed for toxic effects in LCIA (e.g. USEtox™) already use data that are in a form that can be obtained from the REACH information. However, it is highly possible that many of the details needed for REACH (such as the detailed exposure assessments in the CSR) will be confidential, while the results (e.g. use gloves, wear safety glasses) will be public. These results are not information that is typically useful for LCA work.

The intensified work with fate and exposure models that is a result of REACH should provide data that can give

useful input in LCA fate, exposure and effect models. REACH guidance and models (e.g. European Centre for Ecotoxicology and Toxicology of Chemicals, ECETOC 2010) enable the user to specify an activity and risk management measures and thus obtain exposure estimate for workers. This type of information can be a powerful tool for LCA database providers, enabling faster, more standardised estimates of exposure where specific data are not available to the LCA practitioner.

Thus far this section has addressed general similarities and differences between the two approaches for data collection (inventory). The illustrative example (benzene) is a refinery product, which means that there are many interlinked process units. The allocation required is based on physical relationships between the inputs and outputs of the process units relevant to benzene production (EPD 2011). Specific data are used for the transport of crude oil to the refinery and for the refinery process units. Database data are used for the extraction of crude oil and transport of this to the refinery, but data for the relevant mix of crude oil raw materials specifically bought by the refinery in the previous production year are used in order to select the most appropriate data sets. Specific distance data are used, together with database data for oil tankers. Energy data relating to benzene production are based on site-specific data, since the refinery produces its own energy. The study is cradle to gate, but the PCR (EPD 2011) specifies that 500 km of transport to the customer is to be incorporated in the EPD. Thus (for use in the EPD) this product transport distance is set, and inventory data for typical modes of transport are included. As a toxicity assessment (ecotoxicity and human toxicity) is required, the work on data gathering must also focus on the emissions that may contribute to toxic impacts, which may not be commonly included in inventory data sets.

The registration dossier for benzene includes its identity [European Commission (EC) number, EC name, Chemical Abstracts Service (CAS) number, molecular formula, International Union of Pure and Applied Chemistry name, type of substance, trade names and composition]. Physical and chemical properties are given in the dossier (including the sources of these data) as well as environmental fate and pathways, ecotoxicological and toxicological information. Table 1 shows some of this information, alongside analagous data for the USEtox impact assessment model. The registration dossier provides a bank of available test data, including information on the sources, test conditions, test species and whether the tests where performed according to GLP standards. This data bank is the background information for assessment of values to use for toxicity. For example, the dossier gives a PNEC aqua (predicted no effect concentration—freshwater) of 1.9 mg/l for benzene. However, the dossier also contains data on short-term and long-term toxicity to fish, invertibrates, cyanobacteria, microorganisms and other aquatic organisms (found via the menu choices available under ecotoxicological information, see Fig. 1). This underlying toxicity data bank is the basis for the assessments of benzene toxicity and conditions of safe use.

Table 1 provides a summary of the data used for calculation of the characterisation factor for USEtox for benzene (USEtox™ 2010a) alongside the corresponding data given in the benzene registration dossier. It should be noted that data given as “key” data in the dossier are given in this table. The supporting data (not chosen as “key”) are not included, unless otherwise stated. The conclusions from the key data sections of the dossier are given (instead of the more extensive experimental data). The data are presented in the order in which it is given in the USEtox model database. The exceptions to this are for data that are available from the registration dossier, but not in the same form as the USEtox data (e.g. distribution modelling or acute toxicity).

The EC50 values required for USEtox are not specifically given in the dossier (instead LD50 values are the focus). However the underlying databank provides a readily accessible library of relevant toxicity studies. The information about each study includes descriptions of the tests and some detailed data (i.e. species and test conditions), an assessment of the quality of the studies, and the original references. EC50 values can be found in the data bank in some cases or derived from other available data. For example, a spot check on some of the underlying studies for benzene provided EC50 values for aquatic algae/cyanobacteria (growth rate) and for aquatic invertebrates (reproduction) of 100 and 11.6 mg/l, respectively. Benzene is the subject of many supporting studies, providing data for toxicity in the form of no observable effect concentration (NOEC), lowest observed effect concentration, LC50 (median lethal concentration), LC0, EC10, EC20, EC50 and IC50 (the latter being the concentration that induces 50% inhibition of a designated process in an exposed population). This example shows that the greater availability of toxicity data that will result from REACH can provide data to fill gaps in LCIA models.

4.5 Impact assessment

LCIA is a part of the LCA process. Impacts can include toxic effects on human health and ecosystems (e.g. Rosenbaum et al. 2008). Methods for evaluation of human and environmental effects in both approaches are also based on common scientific roots, i.e. EUSES (2010). Physical and chemical properties of the chemicals and experimental data on toxicity are central for both REACH and LCA toxicity assessments. In both cases, these properties (or effects) are combined with

environmental compartment models. The degree of exposure suffered by the relevant recipients is also an important part of the calculations in both approaches. The EUSES risk assessment approach uses information on qualities of recipients, capacity and tolerance. The environmental compartment models (e.g. local, regional, global) are more detailed than those typically used in LCIA (Huijbregts et al. 2000; Van Beelen 2000), although LCIA can in theory handle local levels of detail. There are examples of LCIA approaches that manage this for impacts with localised effects, e.g. acidification and eutrophication (Seppälä et al. 2006; Potting and Hauschild 2006), but this is not the case for toxic effects using ReCiPe and USEtox™. For toxic effects, the simplification process has led to a consensus, a more common ground being found with less detail, between developers of different LCIA methodology for toxic effects. Hauschild et al. (2008) describes the UNEP-SETAC Life Cycle Initiative consensus process and uses a quotation from Antoine de Saint-Exupéry to illustrate this: "Perfection is achieved, not when there is nothing more to add, but when there is nothing left to take away". The focus for the international consensus work was on which model elements contributed the most to the relative magnitude of the LCIA characterisation factors.

A methodological comparison of LCIA [with particular focus on the Danish EDIP method] and risk assessment is presented in Olsen et al. (2001). This comparison was made before the REACH regulation came into force, but the methodological comparisons given here still apply. LCA seeks best estimates and average toxicity (best practise in a comparative framework), whereas conservative estimates and no effect typically are used in (tiered) risk assessment (REACH). This principle is also reflected in the use of the PNEC, which is based on the NOEC in risk assessment, whereas LCIA methods such as USETox and ReCiPe use the hazardous concentration at which 50% of the species is affected (HC50) based on the effect concentration [50% of the test organism is affected (EC50, Olsen et al. 2001; Larsen and Hauschild 2007)]. Olsen et al. (2001) suggested that risk assessment was conservative, while LCA was realistic, which is illustrated by this difference in approach to the toxicity data on which the two approaches are based.

Environmental exposure assessment in REACH is described as encompassing all of the following targets: fresh surface water (including sediment); marine surface water (including sediment); terrestrial ecosystem; top predators via the food chain (secondary poisoning); micro-organisms in sewage treatment systems; atmosphere—mainly considered for chemicals with a potential for ozone depletion, global warming, ozone formation in the troposphere and acidification; and man indirect, i.e. man exposed via the environment. EUSES equations are recommended for the exposure calculations for all of the above targets (ECHA 2010b). There are different LCIA methods for calculating indirect impacts on human health (Goedkoop and Spriensma 2000; Huijbregts et al. 2005a, b), which are also often based on EUSES equations.

Environmental exposure estimation in REACH consists of the same methodological stages as in LCIA. The guidance (ECHA 2010b) describes the main steps as:

- "Estimation of the releases to air, water (either waste water and/or surface water) and soil at local and regional scale;
- Fate and distribution of the releases in environmental compartments (air, soil, surface water, sediment, biota) and sewage treatment plants and
- Calculation of exposure concentrations in/doses for, respectively:

  – Environmental compartments (…), in terms of Predicted Environmental Concentrations (PECs), at both local and regional scales, covering both direct exposure of organisms and exposure via the food chain for predators
  – Man via the environment (…) in terms of human daily intake of the substance through drinking water, fish, leaf crops, root crops, meat and dairy products, at local and regional scale".

This is in line with LCIA methods, such as USEtox™ (Rosenbaum et al. 2008; Hauschild et al. 2008; USEtox™ 2010a), where toxicity impact score (IS_t) is calculated using the general equation $IS_t = \sum_i (CF_{ti} \times M_i)$, where M_i is the mass emitted per emission scenario i, CF_{ti} is the corresponding toxicity characterisation factor summed over all emission scenarios, i. The characterisation factor for a given chemical is a result of its physical and chemical properties combined with its toxicity and exposure calculations (e.g. EUSES equations mentioned above, Rosenbaum et al. 2008).

The environmental exposure estimation guidance also continues with the following information: "Most of the current guidance on environmental exposure estimation has been developed mainly for organic substances. Metals and metal compounds present particularities (natural background and historical releases, speciation, adsorption/desorption behaviour, differences in bioavailability) which require specific adaptations when performing the exposure assessment". These issues are also well known in the LCIA field, e.g. Pizzol et al. (2010) and Rosenbaum et al. (2008).

The previous paragraphs show that the calculation of toxic impacts in REACH and the equivalent potential effects in LCIA correspond with each other. There is significant overlap between the theory behind the two approaches as well as the calculation methods, which can be exploited to the advantage of companies wanting to

streamline their use of resources. The calculations are used for different purposes—in LCIA, comparisons between best estimates and average toxicity, but conservative estimates in REACH—but the principles and data sources are related.

The LCA approach results in midpoint (e.g. 1,4-dichlorobenzene equivalents) or end-point factors (e.g. DALY), i.e. impact potentials or impact scores, whereas REACH information results in advice on RMM. It will require a significant change in mindset for REACH analysts to present toxic effects in a life cycle framework (for example, expressed in terms of DALY). The current perspective is that complying with REACH should reduce the exposure to a level that results in no actual effects. However, the concept of acceptable risk has been accepted elsewhere [for example, in quantitative risk assessment of accident hazards (Marshall and Ruhemann 2001) and risk management (Van Leeuwen and Vermeire 2007)]. Therefore, there is potential for convergence in methods of assessing potential impact.

Thus far this section has addressed general similarities and differences between the two approaches for impact assessment. The following compares specific aspects of impact assessment for the illustrative example. The impact assessment information required for the benzene EPD example is listed in the PCR (EPD 2011) under potential environmental impact. The EPD for benzene shall report the following potential environmental impacts per functional unit: global warming potential (CO_2 equivalents, 100-year perspective), emission of ozone depleting gases (CFC 11 equivalents, 20 years), emission of acidification gases (SO_2 equivalents), emissions of gases that contribute to the creation of ground level ozone (ethene equivalents), emissions of substances to water contributing to oxygen depletion (PO_4^{3-} equivalents) and abiotic depletion potential (kilogram antimony equivalents). The PCR also gives a list of other specific emissions and material flows that shall be reported in the EPD per functional unit. In order to calculate the impacts, the inventory data are used, together with characterisation factors (as described above for USEtox) to calculate impact scores for each impact category. The emissions of all relevant substances included in the inventory would be included in the USEtox toxicity assessment for benzene not just emissions of benzene. The USEtox characterisation factors for benzene [expressed in comparative toxic units (CTU)] are shown in Table 2 (USEtox™ 2010b). The relevant characterisation factor is dependent on the emission compartment and the type of effect (e.g. cancer, non-cancer).

The REACH registration dossier for benzene gives the conclusions of the assessments of the available data for human toxicity and ecotoxicity in the form of classification and labelling (e.g. “H225: Highly flammable liquid and vapour”; “H315: Causes skin irritation”; “H340: May cause genetic defects”; “H372: Causes damage to organs - affected organs: haematopolitic system. Route of exposure: Oral oral, inhalation and dermal”). The hazard classifications are also supplemented by precautionary statements, examples of these for benzene are: “P210: Keep away from heat/sparks/open flames/…/hot surfaces. … no smoking”; “P233: Keep container tightly closed.”; “P260: Do not breathe dust/fume/gas/mist/vapours/spray.”; “P280: Wear protective gloves/protective clothing/eye protection/face protection.”; “P303+P361+P353: if on skin (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower”. The DSD-DPD information is also given in the current dossier, which is the previous system of labelling according to 67/548/EEC Annex 1.

The assessment of impacts required for the REACH CSA for benzene, which connects the detailed physical, chemical and toxicity data described above, with actual releases and recipients, is not publicly available. These assessments are submitted confidentially to ECHA for approval. The publicly available conclusions are for example guidance on safe use, exposure controls and personal protection guidelines, and occupational exposure limits [for benzene these are given as “UK:HSE EH40/2005: Long-term exposure limit (8-h TWA reference period):1 ppm—3.25 mg/m^3; IRL(2002): OEL (8 h): 1 ppm—3.25 mg/m^3; EC (1999): 1 ppm—3.25 mg/m^3; US (ACGIH-2009): TLV-8 h TWA: 0.5 ppm—1.6 mg/m^3; TLV-15 min STEL: 2.5 ppm—8 mg/m^3”]. The information in the guidance documents has been used as the basis for the general similarities and differences for impact assessment described above. The lack of a publicly available CSA means that it is only possible to describe the benzene example in quite general terms. The available information indicates that the release estimation data could be used to check the quality of the existing data for benzene emissions in LCA inventory databases. It is also possible to compare specific data for the fate and distribution models from the CSA with those that USEtox is based upon. If there are data gaps or weaknesses in the USEtox model for benzene, these could be addressed. Similarly if there were difficulties with the CSA fate and distribution models, the USEtox model could supplement the CSA model.

4.6 Interpretation and application

REACH is more obviously applicable to occupational health situations, where risk assessment steps in the REACH guidelines ensure that guidance about appropriate risk management measures (e.g. personal protective equipment) are given in order to minimise potential health effects on workers as well as the environment. Hellweg et al. (2009) summarised the work performed for the UNEP-SETAC Life Cycle Initiative by an international expert

Table 2 USEtox characterisation factors for benzene

Type of toxicity	Emission compartment	Characterisation factor (CTU)	
Human health (cases/kg emitted)	Emission to urban air	Cancer	4.7 E^{-7}
		Non-cancer	1.2 E^{-7}
		Total	5.9 E^{-7}
	Emission to continental scale rural air	Cancer	1.2 E^{-7}
		Non-cancer	3.0 E^{-8}
		Total	1.5 E^{-7}
	Emission to continental scale freshwater	Cancer	2.4 E^{-7}
		Non-cancer	6.1 E^{-8}
		Total	3.0 E^{-7}
	Emission to continental scale sea water	Cancer	2.5 E^{-8}
		Non-cancer	6.3 E^{-9}
		Total	3.1 E^{-8}
	Emission to continental scale natural soil	Cancer	1.1 E^{-7}
		Non-cancer	2.7 E^{-8}
		Total	1.4 E^{-7}
	Emission to continental scale agricultural soil	Cancer	1.3 E^{-7}
		Non-cancer	3.3 E^{-8}
		Total	1.6 E^{-7}
Ecotoxicity (PAF m^3 day/kg emitted)	Emission to urban air		0.064
	Emission to continental scale rural air		0.064
	Emission to continental scale freshwater		65.98
	Emission to continental scale sea water		0.013
	Emission to continental scale natural soil		2.049
	Emission to continental scale agricultural soil		2.049

PAF potentially affected fractions of species

group on the integration of human indoor and outdoor exposure in LCA. This work found that the LCA approach should include a single compartment box for indoor exposure. The comparison between indoor and outdoor human exposure per unit of emission showed that for many pollutants, intake per unit of indoor emission may be several orders of magnitude higher than for outdoor emissions. This work concluded that indoor exposure should be routinely addressed within LCA and highlighted that currently this is not the case. Synergies between REACH and the LCIA part of LCA could provide important methodological development to facilitate inclusion of occupational health aspects in LCA.

If REACH requires a company to consider substitution of a given substance (i.e. a restricted, annex XIV substance) with an alternative and a company wishes to analyse and report the consequences of using an alternative technology (e.g. in order to make a case for authorisation of the substance in opposition to a substitution requirement), a socio-economic analysis is required to support authorisation. "Comparison with risks to the environment from alternative technologies replacing the restricted substance will probably in many cases primarily address changes in the use of other substances in the relevant processes caused by the introduction of the alternative technology" (ECHA 2011b). A potential difficulty with this comparison is described in the guidance as "the risk of toxicity and or risk of persistence in the environment may need to be compared with other kinds of risks. For example such as the risk presented by the generation of greenhouse gases from increased use of energy or risks by increased production of waste etc." The weighting step in LCA methodology addresses this issue and could prove useful for the comparison of alternatives where changes in different types of impacts need to be compared.

The combination of LCA and REACH can be used to aid companies in strategic decisions. Research linking LCA and REACH information for products, based on a functional perspective, could lead to a powerful product innovation tool. Data about these two different aspects can be used, as for traditional LCA information, to drive change and improvement (Baumann and Tillman 2004, pp. 20–21). The work performed in the Innochem project linking these two key issues (REACH and LCA) has provided valuable

input to the companies' innovation processes (Hanssen 2010), illustrating the practical value of this approach. Exemplification of linking LCA and REACH information about products, in order to drive a more optimal product innovation process, will form the basis of further work in the Innochem project and further publications from the project team. Presently this work is focussing on coatings for the furniture and offshore industries.

5 Conclusions

REACH and LCA approaches are by nature different in scope and framework, but focus on some of the same issues. Many companies will use both approaches, which may result in synergies but also contradictory results. This can be problematic for decision makers in companies involved with development of new products or redesign of existing ones. Bearing in mind the viewpoint of both approaches and therefore paying greater attention to each approach in its intended area of application will ensure that decision makers are aware of potential conflicts during the product development process. They may therefore be able to seek solutions that will avoid these conflicts of interest.

The greater availability of toxicity data that will result from REACH should strengthen LCA toxicity results and methods by providing more data about the toxicological effects of chemicals. This will contribute to increasing knowledge about fate and exposure models and effects, as well as easing the data availability problems when calculating characterisation factors using models like USEtox™.

The implementation of REACH could also greatly benefit from the functional approach used in LCA. A functional approach can be essential, particularly when questions about substitution arise. If REACH is implemented in companies without exploiting the functional and life cycle approach and potential synergies with LCA, this could lead to suboptimal solutions. LCA has been identified as a potentially appropriate method within the socio-economic assessment needed for the authorisation process (Christensen et al. 2003). The guidelines for the authorisation process (ECHA 2011b) state that LCA is appropriate for comparing risks in complex systems, considering more far-reaching impacts from the whole life cycle of products. The guidance states that use of LCA "may make it difficult to focus only on the impacts from the alternative since the LCA is concerned with all impacts from the final end product". LCA is described as designed more for selection of the sustainable manufacture and use of products than selecting lower risk alternatives for hazardous chemicals for particular uses. However, the guidance also states "but the same basic methods and approaches used in LCA to describe the effects could be used".

Several examples of synergies between REACH and LCA are presented in Section 4 of this paper. The theory behind the calculation of toxic impacts in LCIA, REACH as well as the calculation methods have a lot of concurrance, which can be exploited to the advantage of companies wanting to streamline their use of resources. Data requirements for both REACH and LCA can be aided by exploiting each other's guidance documents and databases. Thus implementation of REACH and the associated methodological guidelines can provide sources of data that can fill data gaps in LCIA and also strengthen LCIA methodology. The examples here show perhaps clearer indications of how REACH can strengthen LCIA, but further work from the Innochem project will illustrate more specifically how exploitation of the LCA approach can also strengthen REACH implementation in companies. It seems to be clear that LCA tools can be used to improve the environmental assessments required for REACH. Exploitation of REACH information together with LCA information in order to drive more optimal product development will be considered. Here, "optimal" refers to several aspects, including both environmental and resource efficiency for the environment as a whole and compliance with REACH.

LCA methodology is also often used by companies to focus on improvements of product systems. This is an aspect of LCA methodology that could provide positive influence on REACH implementation by contributing to an innovative improvement perspective. Thus combining aspects of LCA with REACH can give companies a competitive edge and benefit society.

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